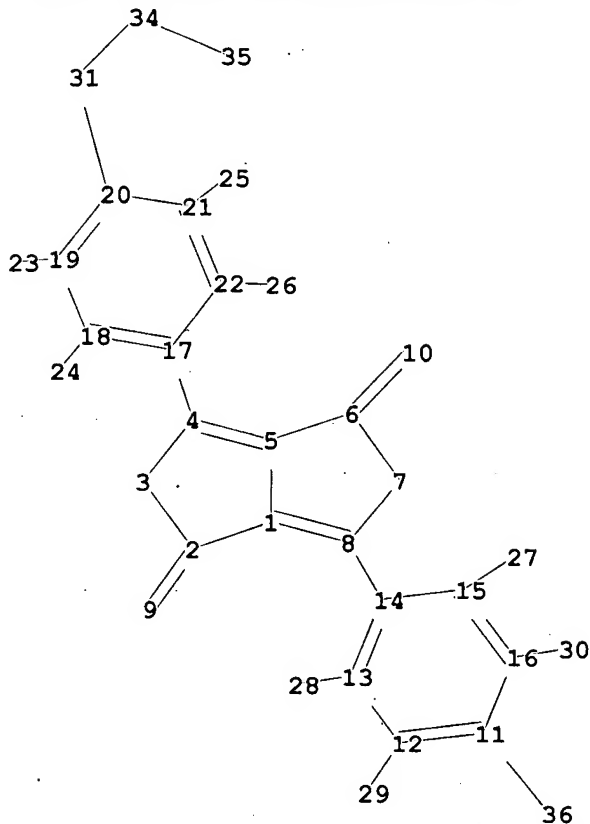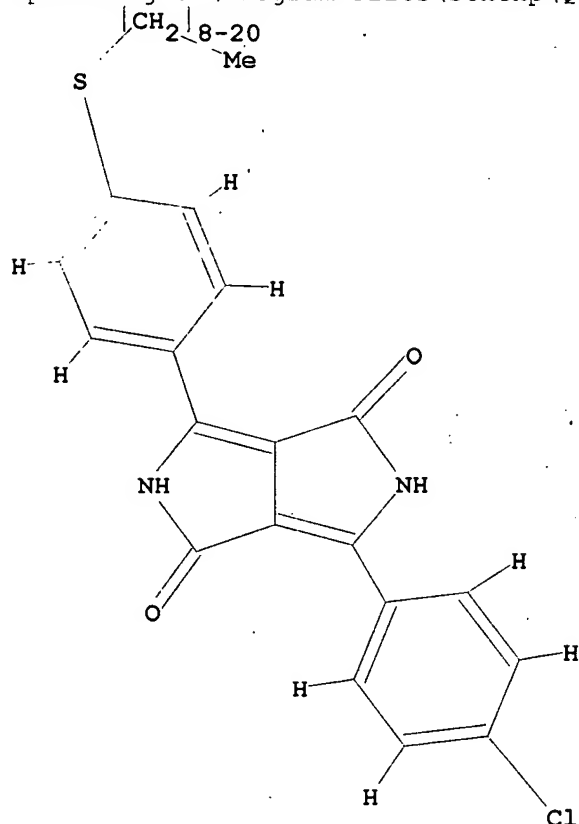Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION3.str

chain nodes :
9 10 23 24 25 26 27 28 29 30 31 34 35 36
ring nodes :
1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25
22-26 31-34 34-35
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16
17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 20-31
exact bonds :
4-17 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34
34-35
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS
34:CLASS 35:CLASS 36:CLASS

July 17, 2007

L10   STRUCTURE UPLOADED

=> s l10 full
FULL SEARCH INITIATED 11:02:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   66 TO ITERATE

100.0% PROCESSED   66 ITERATIONS   2 ANSWERS
SEARCH TIME: 00.00.01

L11   2 SEA SSS FUL L10

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                              ENTRY   SESSION
FULL ESTIMATED COST   172.10   864.35

FILE 'CAPLUS' ENTERED AT 11:02:55 ON 16 JUL 2007
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FILE LAST UPDATED: 15 Jul 2007 (20070715/ED)

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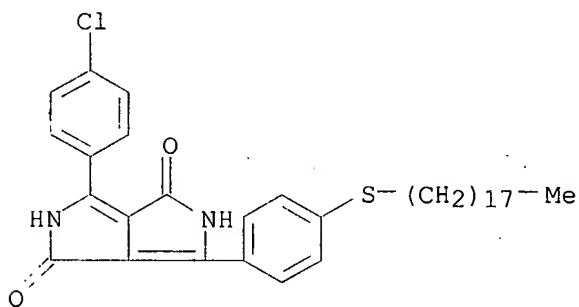
=> s l11
L12   1 L11

=> d ibib hitstr 1

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:395400 CAPLUS <<LOGINID::20070716>>
DOCUMENT NUMBER: 142:412928
TITLE: Heat-stable diketopyrrolopyrrole pigment mixtures for
                        cosmetics
INVENTOR(S):   Wallquist, Olof; Lenz, Roman; Feiler, Leonhard;
                        Dueggeli, Mathias; Yousaf, Taher; De Keyzer, Gerardus
PATENT ASSIGNEE(S):   Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 54 pp.
                        CODEN: PIXXD2
DOCUMENT TYPE: Patent
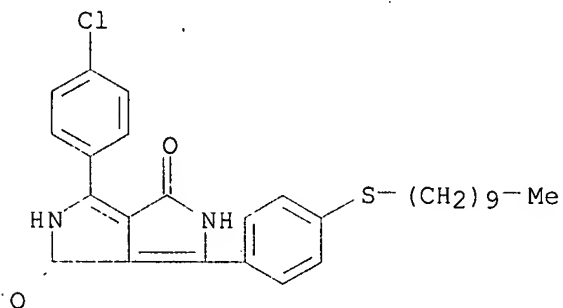LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005040284	A1	20050506	WO 2004-EP52426	20041004

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004284235	A1	20050506	AU 2004-284235	20041004
CA 2542519	A1	20050506	CA 2004-2542519	20041004
EP 1675916	A1	20060705	EP 2004-791138	20041004

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1871309	A	20061129	CN 2004-80031296	20041004
BR 2004015831	A	20070102	BR 2004-15831	20041004
JP 2007514798	T	20070607	JP 2006-536078	20041004
US 2007028807	A1	20070208	US 2006-576703	20060419
IN 2006CN01381	A	20070706	IN 2006-CN1381	20060421

PRIORITY APPLN. INFO.:   CH 2003-1817   A 20031023
                                          WO 2004-EP52426   W 20041004

OTHER SOURCE(S):   MARPAT 142:412928
IT   850566-77-7P
    RL: COS (Cosmetic use); IMF (Industrial manufacture); MOA (Modifier or
    additive use); TEM (Technical or engineered material use); BIOL
    (Biological study); PREP (Preparation); USES (Uses)
        (dark red pigment; production of heat-stable diketopyrrolopyrrole pigment
        mixts. for cosmetics)
RN   850566-77-7 CAPLUS
CN   Pyrrolo[3,4-c]pyrrole-1,4-dione, 3-(4-chlorophenyl)-2,5-dihydro-6-[4-
     (octadecylthio)phenyl]- (9CI) (CA INDEX NAME)

IT   850566-80-2P
    RL: COS (Cosmetic use); IMF (Industrial manufacture); MOA (Modifier or
    additive use); TEM (Technical or engineered material use); BIOL
    (Biological study); PREP (Preparation); USES (Uses)
        (red pigment; production of heat-stable diketopyrrolopyrrole pigment mixts.
        for cosmetics)
RN   850566-80-2 CAPLUS

July 17, 2007

CN   Pyrrolo[3,4-c]pyrrole-1,4-dione, 3-(4-chlorophenyl)-6-[4-
      (decylthio)phenyl]-2,5-dihydro- (9CI)   (CA INDEX NAME)

REFERENCE COUNT: 20   THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
                                  RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                    ENTRY   SESSION
FULL ESTIMATED COST   4.09   868.44

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DICTIONARY FILE UPDATES: 15 JUL 2007 HIGHEST RN 942400-66-0

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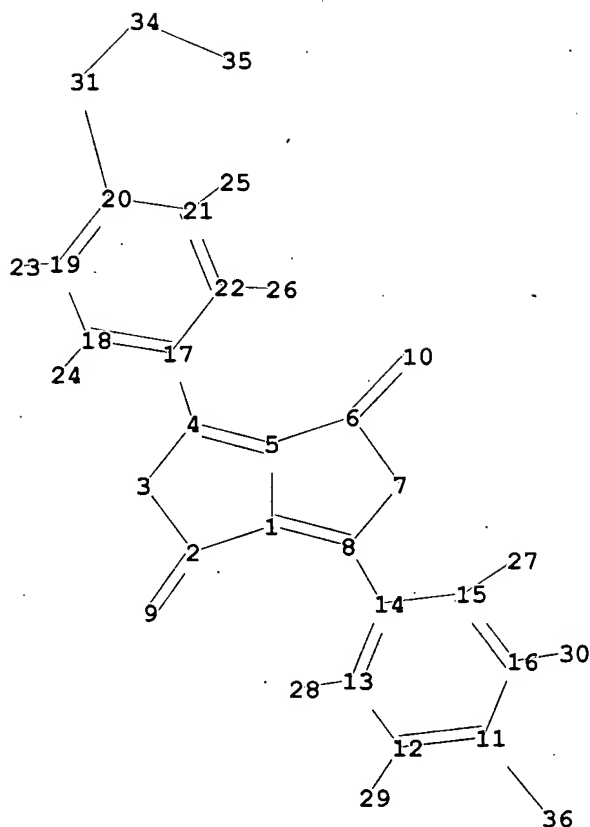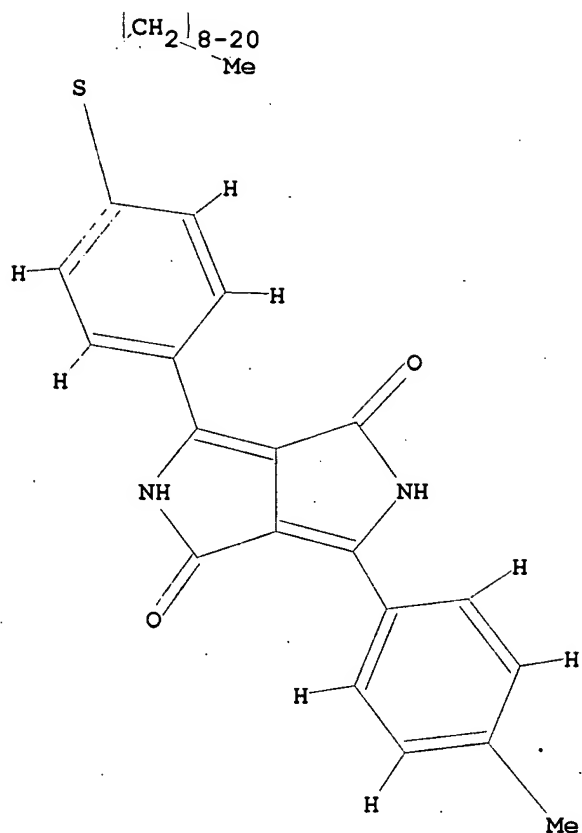TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION4.str

July 17, 2007

chain nodes :
9 10 23 24 25 26 27 28 29 30 31 34 35 36
ring nodes :
1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25
22-26 31-34 34-35
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16
17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 20-31
exact bonds :
4-17 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34
34-35
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS
34:CLASS 35:CLASS 36:CLASS

July 17, 2007

L13   STRUCTURE UPLOADED

=> s l13 full
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FULL SCREEN SEARCH COMPLETED -   66 TO ITERATE

100.0% PROCESSED   66 ITERATIONS   2 ANSWERS
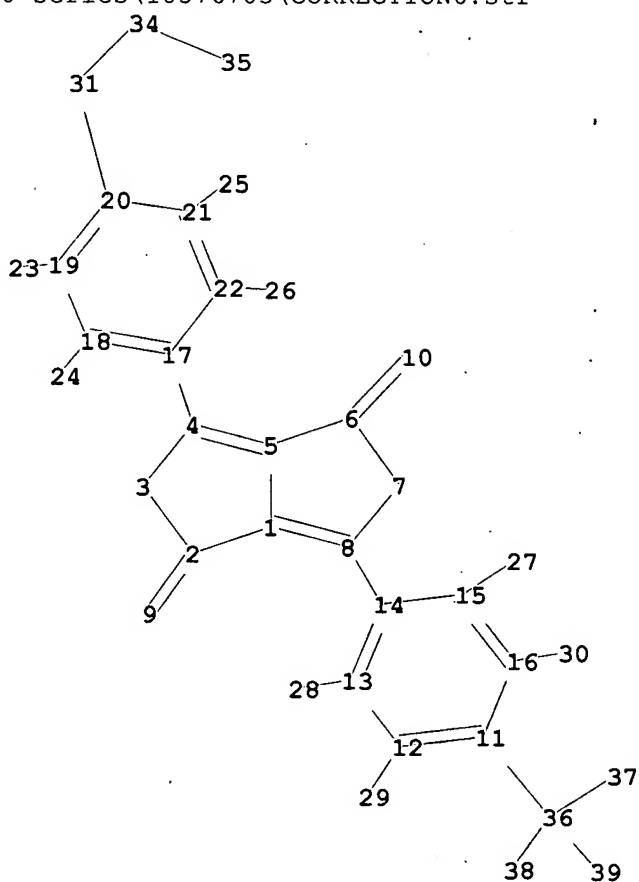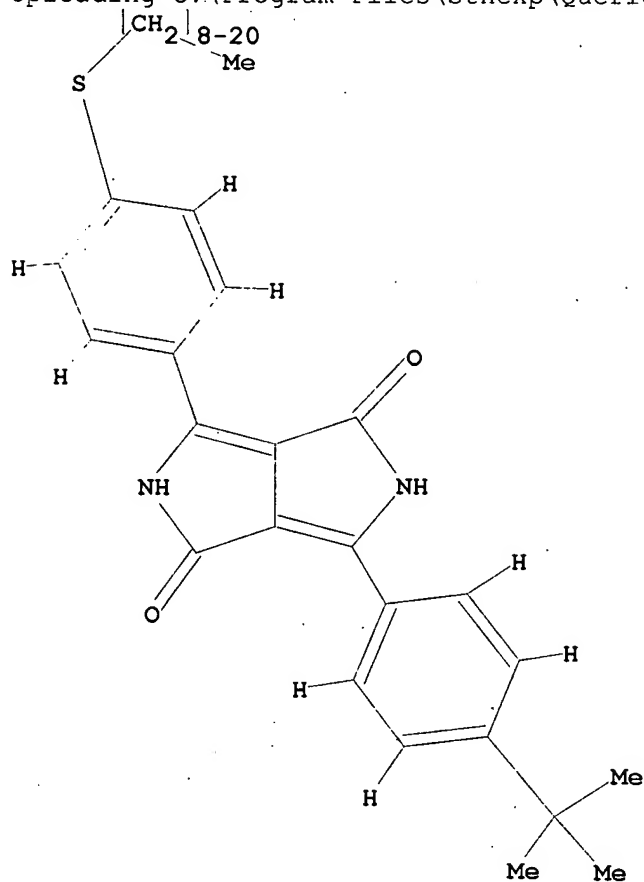SEARCH TIME: 00.00.01

L14   2 SEA SSS FUL L13

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION6.str

chain nodes :
9 10 23 24 25 26 27 28 29 30 31 34 35 36 37 38 39
ring nodes :
1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25
22-26 31-34 34-35 36-37 36-38 36-39
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16
17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 20-31
exact bonds :
4-17 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34

July 17, 2007

10/576,703 REACTION SEARCH.

34-35 36-37 36-38 36-39
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21. 21-22

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS
34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS

L15   STRUCTURE UPLOADED

=> s l15 full
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FULL SCREEN SEARCH COMPLETED -   151 TO ITERATE

100.0% PROCESSED   151 ITERATIONS   1 ANSWERS
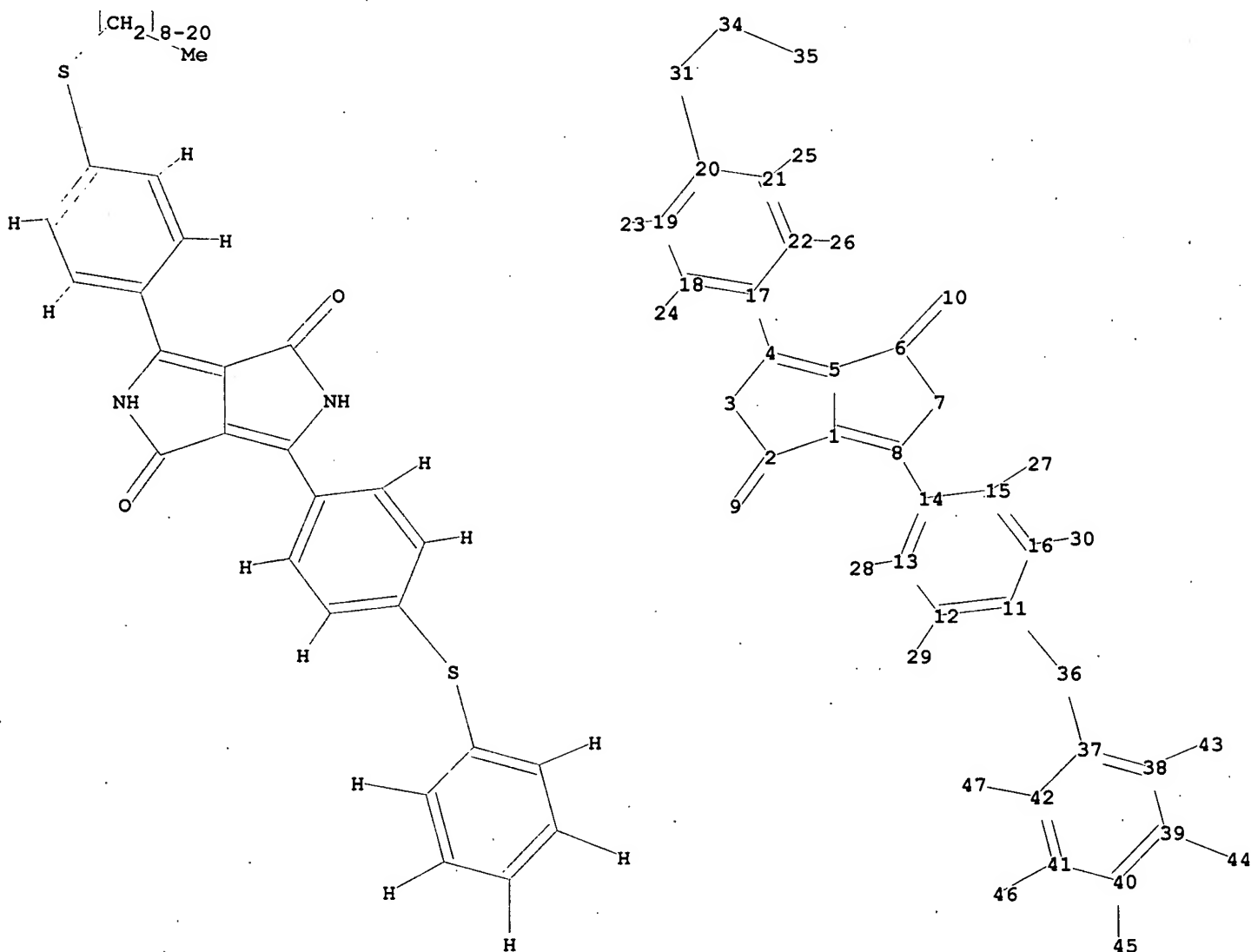SEARCH TIME: 00.00.01

L16   1 SEA SSS FUL L15

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION7.str

July 17, 2007

chain nodes :
9   10   23   24   25   26   27   28   29   30   31   34   35   36   43   44   45   46   47
ring nodes :
1   2   3   4   5   6   7   8   11   12   13   14   15   16   17   18   19   20   21   22   37   38   39
40   41   42
chain bonds :
2-9   4-17   6-10   8-14   11-36   12-29   13-28   15-27   16-30   18-24   19-23   20-31   21-25
22-26   31-34   34-35   36-37   38-43   39-44   40-45   41-46   42-47
ring bonds :
1-2   1-5   1-8   2-3   3-4   4-5   5-6   6-7   7-8   11-12   11-16   12-13   13-14   14-15   15-16
17-18   17-22   18-19   19-20   20-21   21-22   37-38   37-42   38-39   39-40   40-41   41-42
exact/norm bonds :
1-2   1-5   1-8   2-3   2-9   3-4   4-5   5-6   6-7   6-10   7-8   11-36   20-31   36-37
exact bonds :
4-17   8-14   12-29   13-28   15-27   16-30   18-24   19-23   21-25   22-26   31-34   34-35
38-43   39-44   40-45   41-46   42-47
normalized bonds :
11-12   11-16   12-13   13-14   14-15   15-16   17-18   17-22   18-19   19-20   20-21   21-22
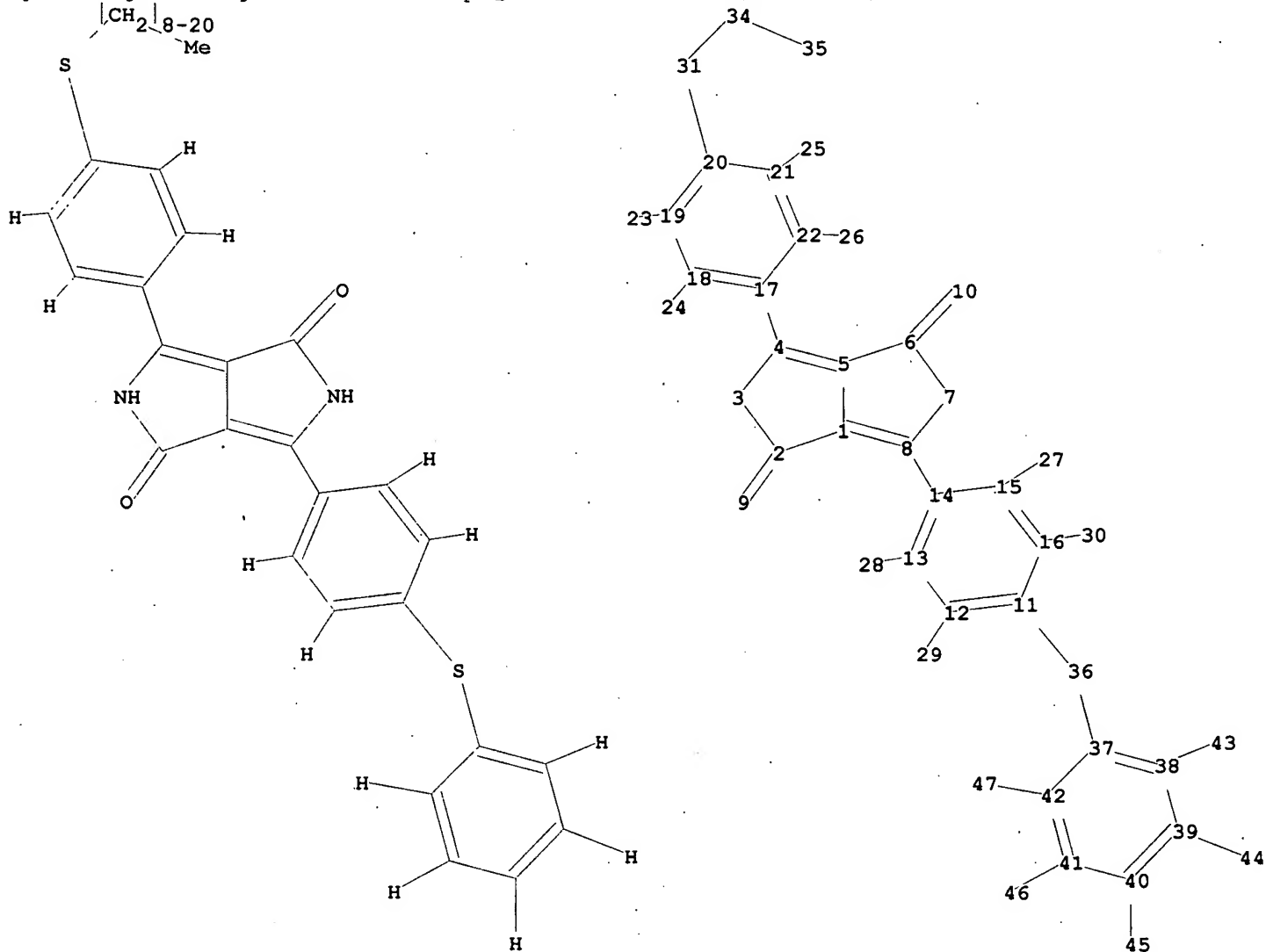37-38   37-42   38-39   39-40   40-41   41-42

July 17, 2007

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS
34:CLASS 35:CLASS 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom
43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\CORRECTION7.str

July 17, 2007

chain nodes :
9 10 23 24 25 26 27 28 29 30 31 34 35 36 43 44 45 46 47
ring nodes :
1 2 3 4 5 6 7 8 11 12 13 14 15 16 17 18 19 20 21 22 37 38 39
40 41 42
chain bonds :
2-9 4-17 6-10 8-14 11-36 12-29 13-28 15-27 16-30 18-24 19-23 20-31 21-25
22-26 31-34 34-35 36-37 38-43 39-44 40-45 41-46 42-47
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16
17-18 17-22 18-19 19-20 20-21 21-22 37-38 37-42 38-39 39-40 40-41 41-42
exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 5-6 6-7 6-10 7-8 11-36 20-31 36-37
exact bonds :
4-17 8-14 12-29 13-28 15-27 16-30 18-24 19-23 21-25 22-26 31-34 34-35
38-43 39-44 40-45 41-46 42-47
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
37-38 37-42 38-39 39-40 40-41 41-42

G1:X,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS
34:CLASS 35:CLASS 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom
43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS

L17   STRUCTURE UPLOADED

=> s l17 full
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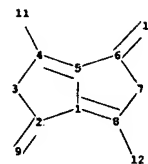FULL SCREEN SEARCH COMPLETED -   67 TO ITERATE

100.0% PROCESSED   67 ITERATIONS   1 ANSWERS
SEARCH TIME: 00.00.01

L18   1 SEA SSS FUL L17

July 17, 2007

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\RXN2222222222222222.str

chain nodes :
9 10 11 12 22 23 24 27
ring nodes :
1 2 3 4 5 6 7 8 16 17 18 19 20 21
chain bonds :
2-9 4-11 6-10 8-12 17-27 20-22 22-23 23-24
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 20-22
exact bonds :
17-27 22-23 23-24
normalized bonds :
16-17 16-21 17-18 18-19 19-20 20-21

G1:H,CH3,CF3,CN,X

G2:C,S,N

G3:Cb,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
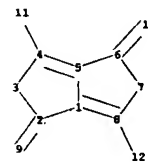11:Atom 12:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom 20:CLASS 21:Atom 22:CLASS
23:CLASS 24:CLASS
27:CLASS

L1   STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\RXN22.str

July 17, 2007

chain nodes :
9 10 11 12 22 23 24 27
ring nodes :
1 2 3 4 5 6 7 8 16 17 18 19 20 21
chain bonds :
2-9 4-11 6-10 8-12 17-27 20-22 22-23 23-24
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 20-22
exact bonds :
17-27 22-23 23-24
normalized bonds :
16-17 16-21 17-18 18-19 19-20 20-21

G1:H,CH3,CF3,CN,X.

G2:C,S,N

G3:Cb,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom 20:CLASS 21:Atom 22:CLASS
23:CLASS 24:CLASS
27:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 16

L2   STRUCTURE UPLOADED

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SCREENING COMPLETE -   0 REACTIONS TO VERIFY FROM   0 DOCUMENTS

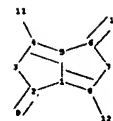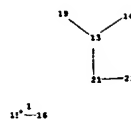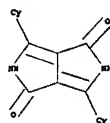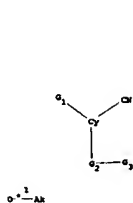100.0% DONE   0 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.01

L3   0 SEA SSS FUL L2 (0 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\RXN111111.str

July 17, 2007

chain nodes :
9 10 11 12 13 14 15 16 19 21 23
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
2-9 4-11 6-10 8-12 13-14 13-19 13-21 15-16 21-23
ring bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8
exact/norm bonds :
1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 13-14 13-19
13-21 15-16 21-23

G1:H,CH3,CF3,CN,X,[*1]

G2:C,S,N

G3:Cb,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 19:CLASS 21:CLASS 23:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 13

L4   STRUCTURE UPLOADED

July 17, 2007

10/576,703   REACTION SEARCH

=> d
L4 HAS NO ANSWERS
L4   STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE. ***

Structure attributes must be viewed using STN Express query preparation.

=> s l4 full
FULL SEARCH INITIATED 13:57:03 FILE 'CASREACT'
SCREENING COMPLETE -   2423 REACTIONS TO VERIFY FROM   251 DOCUMENTS

100.0% DONE   2423 VERIFIED   5 HIT RXNS   3 DOCS
SEARCH TIME: 00.00.03

L5   3 SEA SSS FUL L4 (5 REACTIONS)

July 17, 2007

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L2	111	548/453.ccls. and pigment	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/07/17 09:57
L3	77	L2 and diketopyrrolopyrrole	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/07/17 09:57